Continuum contact mechanics theories at the atomic scale

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Continuum contact mechanics theories at the atomic scale: an investigation on non-adhesive contacts

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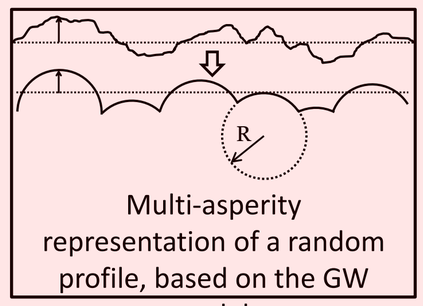
Introduction: surface roughness at the atomic scale

Surface roughness, which is always present in some length scales, has a major impact on most tribology-related studies. This is mainly because it can alter the surface forces, which are dominant at the nanoscale, and influence the functionality of micro and nano-sized devices; in fact, contact itself is initiated at the atomic scale. Considering the breakdown of the macroscopic laws of friction at the atomic scale, numerical simulations, such as molecular dynamics (MD), are used to study these systems. Surfaces in nature and engineering applications have random roughness that can be described as being fractal; however, many analytical models, such as those based on the Greenwood-Williamson (GW) model [1], treat roughness as a statistical collection of parabolic asperities.

In the GW model, the tallest peak is assumed to make the first contact, which resembles a sphere-on-flat contact. The tip of each peak can be modelled as a sphere such that analytical solutions can be derived from sphere-on-flat geometries, e.g. the Hertzian solution.

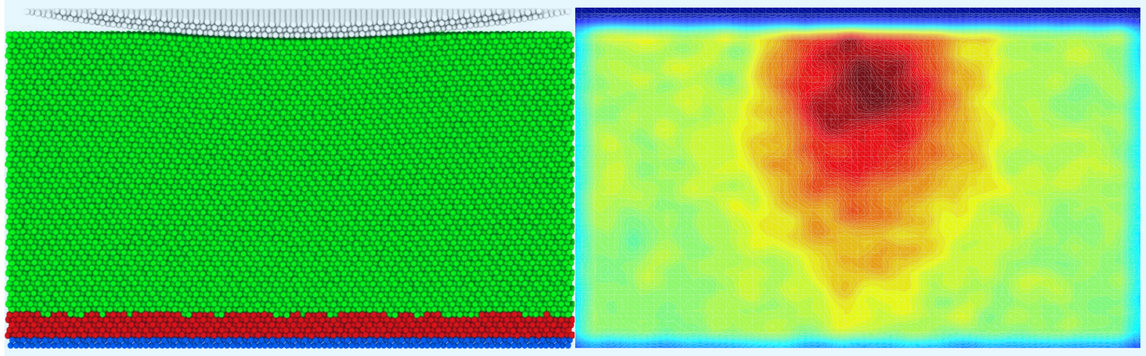


Multi-asperity representation of a random profile, based on the GW model.

Here, we present our results on the normal contacts of the non-adhesive sphere-on-flat problem, and compare the results of two cases of rough surface contact. Simulations were performed using LAMMPS [2], and visualized via OVITO [3].

Atomistic Hertzian Contact

The Hertz contact theory was examined by studying the pressure distribution of the non-adhesive contact between a number of spherical rigid indenters with different sizes, ranging between 15 Å and 1000 Å, on a deformable atomically flat substrate [4]. The system was generated from calcium atoms, at 300 K.



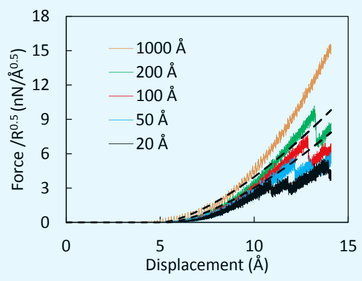
Contacting system: (Left) A spherical cap indenter of $\mathrm{R} = 1000$ Å indents an atomically flat substrate. The blue, red, green, and white dots represent the fixed, thermostatic, Newtonian, and indenter atoms. **(Right)** The system's responses were collected up to the point before which the stress fields were affected by the boundaries.

Deviations between MD results and Hertz

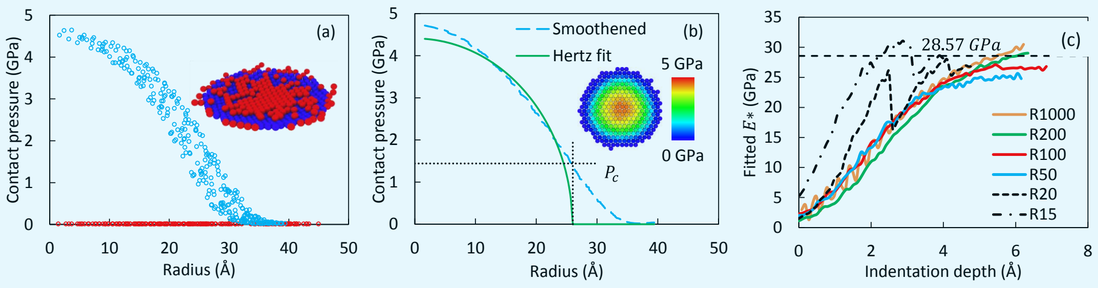
Based on the Hertz theory force can be described as:

$F_H = \frac{4}{3} E^* R^{0.5} d^{1.5}$, with $E^* = \left(\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}\right)^{-1}$, and

R: Indenter's radius, d: Indentation depth, E_i: Elastic modulus, ν_i: Poisson's ratio. The applicability of this method was investigated through the pressure distribution at the contacts.



Pressure distribution at the contact



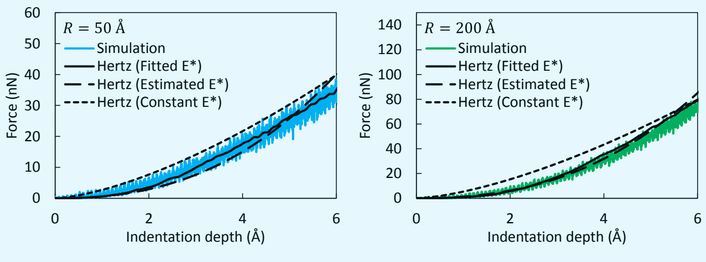
(a, b) The interacting atoms were detected by a non-zero pressure criterion. The Hertz formula was fitted to the smoothened data, only after the background noise was removed with a threshold of $0.02\ GPa$.

(c) The Hertz theory describes the pressure distribution as $p(r) = p_0(1 - (r/r_c)^2)^{0.5}$, where p_0 is the maximum pressure, and r_c is the contact radius. These values were used for estimating the reduced modulus $E^* = \frac{\pi}{2} p_0 \frac{R}{r_c}$. The results showed that the fitted values of E^* vary with indentation depth for shallow indentations, and tend toward the reduced Young's modulus of calcium, i.e. $E^* = 28.57\ GPa$ that is calculated based on the employed potential energy. Note that the jaggedness of the results of 15 Å and 20 Å is due to the inevitable stepped geometry of the smaller indenters.

Redefinition of E^*

Based on the results, it is proposed that: $E^*_{estimated} = C + AR^{B-1}\, d$, with $0 \le d \le 4$Å, and A, B, and C being constants.

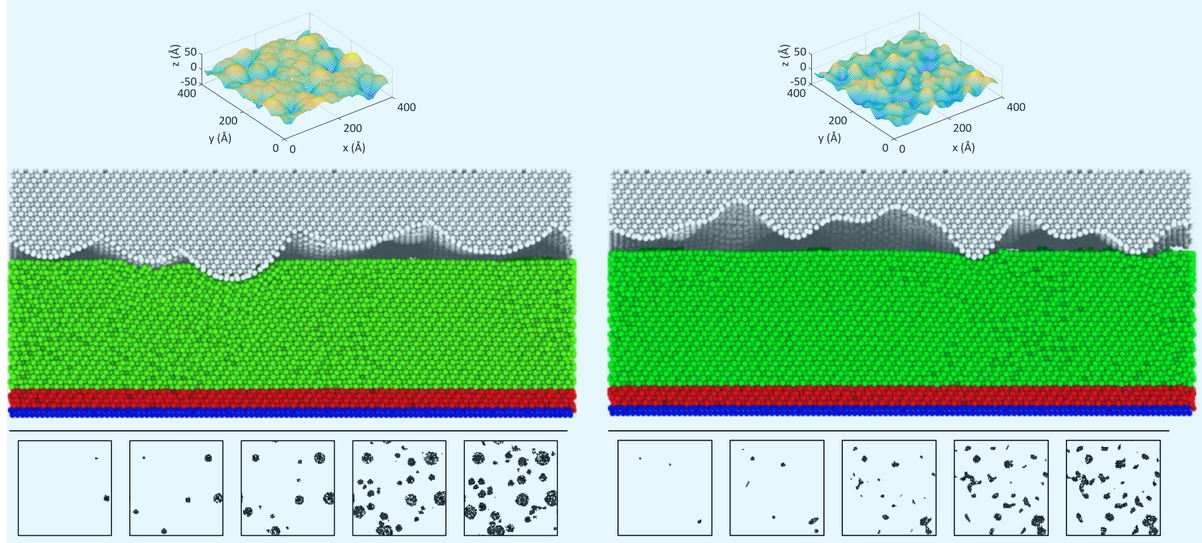
Comparisons between the force-indentation curves show the effects of using different values of $E^*$for the Hertz theory: Fitted E^*, $E^*_{estimated}$, and $E^*_{constant} = 28.57\ GPa$.



Atomistic Rough Surface Contact

The contacts of two comparable rough surfaces were simulated: one GW surface, and one randomly rough (RR) one [4]. For the both surfaces, the mean radius of curvature was estimated to be ~ 110 Å. Using the rough surfaces, two rough atomistic blocks were generated, and their contact with an atomically flat substrate was simulated.

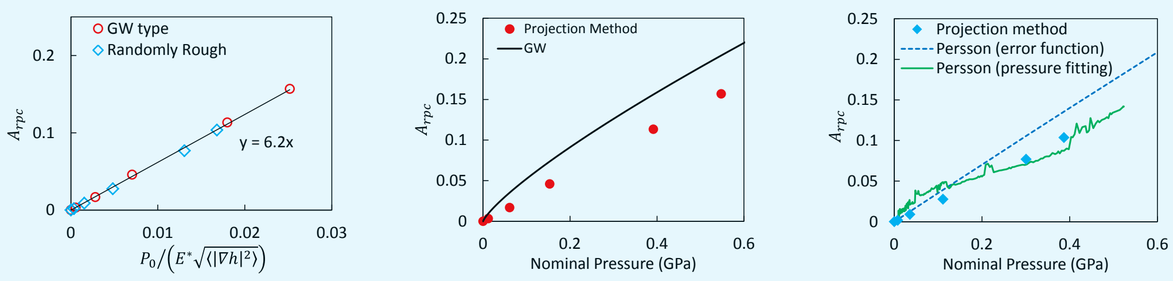
GW rough surface | **RR rough surface**



Contact Evolution: The black dots indicate the contacted atoms of the rough surface contacts at different nominal pressure values.

Rough surface contact mechanics: GW & Persson

In order to study the contact behavior of the simulated systems, two continuum contact mechanics theories, namely Greenwood-Williamson (GW) and Persson [5], were considered. The relation between the relative projected contact area A_{rcp} and the nominal pressure was studied. The solutions of the models were compared with the simulation results.



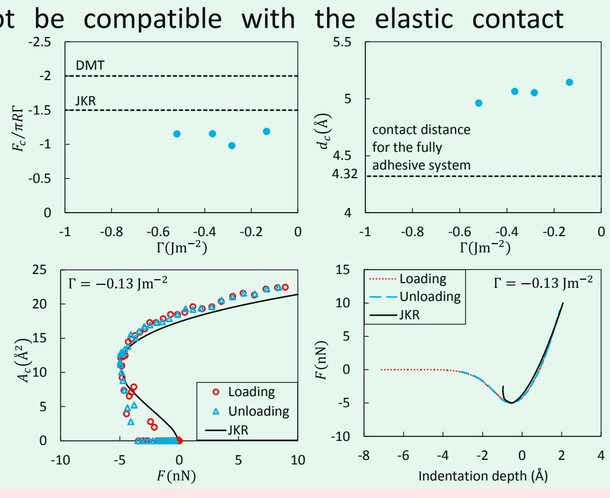
The values of A_{rcp} for both systems showed the same dependence on normalized pressure. Moreover, the results show that the studied rough surface contact theories underestimate the contact areas; however, the Persson theory resulted in closer estimations for A_{rcp} calculated based on fitting the interfacial pressure distribution.

Adhesive contacts: sphere-on-flat problem

In order to study the adhesive MD simulated systems by means of continuum mechanics, the contact distance d_c needs to be calibrated first. It has been shown that, for fully adhesive systems, d_c can be defined using the radial distribution function; however, the adhesion needs to be low enough to prevent the atoms' transfer process and plastic deformation. Otherwise, the simulated systems would not be compatible with the elastic contact mechanics theories.

Initial findings:

1. For the calcium system, the ratio of $F_c/\pi R\Gamma$ was found to be beyond the JKR limit.
2. The JKR theory can be used for calibrating the contact distance. Moreover, this theory can properly describe the contact behavior for loads equal to or greater than the critical load.



Future work

Future studies will focus on randomly rough surface contacts in dry /lubricated conditions.

References: **[1]** Greenwood and Williamson (1966) Proceedings of the Royal Society of London A **295**, p. 300. **[2]** Plimpton (1995) Journal of Computational Physics **117**, p. 1. **[3]** Stukowski (2010) Modelling and Simulation in Materials Science and Engineering **18**, p. 015012. **[4]** Solhjoo and Vakis (2016) Journal of Applied Physics **120**, p. 215102. **[5]** Persson (2001) Journal of Chemical Physics **115**, p. 3840.